

## CLAIMS

1. A method for metabolomically facilitating the diagnosis of a disease state of a subject, comprising:
- 5 obtaining a small molecule profile from a subject suspected of having and/or having a disease state; and
- comparing the small molecule profile from the subject to a standard small molecule profile, thereby diagnosing the disease state.
- 10 2. A method for metabolomically predicting whether a subject is predisposed to having a disease state, comprising:
- obtaining a small molecule profile from the subject; and
- comparing the small molecule profile from the subject to a standard small molecule profile, thereby predicting whether a subject is predisposed to having a disease
- 15 state.
3. A method for metabolomically predicting a subject's response to a therapeutic agent, comprising:
- obtaining a small molecule profile from the subject;
- 20 comparing the small molecule profile of the subject to a known standard established for the therapeutic agent as an indication of whether the subject would benefit from treatment with the therapeutic agent, thereby predicting a subject's response to said therapeutic agent.
- 25 4. A method for metabolomically monitoring the effectiveness of a therapeutic agent in clinical trials, comprising:
- obtaining a small molecule profile from a subject in a clinical trial being treated with a therapeutic agent; and
- monitoring changes in the small molecule profile of the subject as an
- 30 indication of the effectiveness of the therapeutic agent in the subject, thereby monitoring the effectiveness of said therapeutic agent.
5. The method of any one of claims 1-4, wherein said subject is a human.
- 35 6. The method of any one of claims 1-4, wherein said subject is suffering or suspected of suffering from a disease state.

7. The method of any one of claims 1-4, wherein said subject is suffering from an immunological, neurological, metabolic, oncological, viral, or a cardiovascular disorder.
8. A method for generating a small molecule profile of a cellular compartment, comprising:  
obtaining said cellular compartment from a source;  
analyzing said sample to determine the identity of the small molecules in said cellular compartment, thereby generating a small molecule profile of said cellular compartment.
9. The method of claim 8, wherein said cellular compartment is a cell.
10. The method of claim 8, wherein said cellular compartment is the nucleus.
11. The method of claim 8, wherein said cellular compartment is the mitochondria.
12. The method of claim 8, wherein the method for analyzing the sample is selected from the group consisting of HPLC, TLC, electrochemical analysis, mass spectroscopy, refractive index spectroscopy (RI), Ultra-Violet spectroscopy (UV), fluorescent analysis, radiochemical analysis, Near-InfraRed spectroscopy (Near-IR), Nuclear Magnetic Resonance spectroscopy (NMR), and Light Scattering analysis (LS).
13. The method of claim 12, wherein the method for analyzing the sample comprises two or more methods.
14. The method of claim 8, wherein at least 50% of the small molecules of the cellular compartment are identified.
15. The method of claim 14, wherein at least 70% of the small molecules of the cellular compartment are identified.
16. The method of claim 8, wherein the cellular compartment is derived from a healthy cell.

17. The method of claim 8, wherein the source of the cellular compartment is a diseased cell.

18. The method of claim 8, wherein the source of the cellular compartment is suffering from an immunological, metabolic, cardiovascular, neurological, oncological, or viral disorder.

19. The method of claim 8, wherein the source of the cellular compartments are selected from a subject's liver, heart, muscle, brain, nerve, stomach, pancreas, colon, bone, blood, or other tissue.

20. A method for identifying disease relevant small molecules comprising:  
obtaining a small molecule profile of a diseased cellular compartment; and  
comparing the small molecule profile of said diseased cell to a standard small molecule profile;  
thereby, identifying the disease relevant small molecules in said diseased cellular compartment.

21. The method of claim 20, wherein said diseased cellular compartment is a cell.

22. The method of claim 20, wherein said diseased cellular compartment is mitochondria.

23. The method of claim 20, wherein said diseased cellular compartment are nuclei.

24. The method of claim 20, wherein said diseased cellular compartment is obtained from a source suffering from an immunological, metabolic, cardiovascular, neurological, oncological, or viral disorder.

25. The method of claim 20, wherein said diseased cellular compartment is obtained from a human.

26. The disease relevant small molecules identified by the method described in claim 20.

27. A method for identifying small molecules affected by an agent comprising:

- 5 obtaining a small molecule profile of said cellular compartment  
treated with an agent, and  
comparing said small molecule profile to a standard small  
molecule profile;  
thereby, identifying the compounds affected by said agent in said  
cellular compartment.

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28. The method of claim 27, wherein said agent is a toxin.

29. The method of claim 27, wherein said agent is a therapeutic agent.

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30. The method of claim 29, wherein said therapeutic agent is a therapeutic agent used for the treatment of a metabolic, immunological, neurological, oncological, viral, or other disorder.

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31. The method of claim 27, wherein said cellular compartment is obtained from a patient.

32. The method of claim 31, wherein said patient is suffering from a metabolic, immunological, neurological, oncological, viral, or other disorder.

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33. The method of claim 27, wherein said cellular compartment is a cells.

34. The method of claim 27, wherein said cellular compartment is mitochondria.

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35. The method of claim 27, wherein said cellular compartment is a nucleus.

36. The method of claim 27, wherein said small molecule profiles are obtained using one or more of the following: HPLC, TLC, electrochemical analysis, mass spectroscopy, refractive index spectroscopy (RI), Ultra-Violet spectroscopy (UV),  
35 fluorescent analysis, radiochemical analysis, Near-Infrared spectroscopy (Near-IR), Nuclear Magnetic Resonance spectroscopy (NMR), and Light Scattering analysis (LS).

37. A method for identifying small molecules regulated, modulated, or associated with a gene, comprising:

obtaining a small molecule profile of a cellular compartment from a genetically modified source; and

5 comparing the small molecule profile to a standard small molecule profile, thus identifying the small molecules regulated, modulated or associated with the gene.

38. The method of claim 37, wherein said cellular compartment is a cells.

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39. The method of claim 37, wherein said cellular compartment is a mitochondria.

40. The method of claim 37, wherein said cellular compartments is a nucleus.

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41. The method of claim 37, wherein said genetic modification is an expression vector.

42. The method of claim 41, wherein said expression vector is a portion of the human genome.

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43. The method of claim 42, wherein said expression vector is associated with a particular disease state.

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44. A method for identifying potential cell drug targets, comprising: contacting a labeled disease relevant small molecule with cellular components; and

identifying interactions between said cell components and the labeled disease-relevant small molecule, thus identifying potential cell drug targets.

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45. The method of claim 44, wherein said cellular components are a nucleic acid array.

46. The method of claim 44, wherein said cellular components are a protein array.

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47. The cellular components identified by the method of claim 44.

48. A library of small molecules of a cellular compartment of a cell comprising a searchable array of samples of small molecules from a cellular compartment.
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49. The library of claim 48, wherein said small molecules are isolated.
50. The library of claim 48, wherein said cell is an animal cell.
- 10 51. The library of claim 48, wherein said cellular compartment is a mitochondria.
52. The library of claim 48, wherein said cellular compartment is a nucleus.
- 15 53. The library of claim 48, wherein said cellular compartment is a chloroplast.
54. A method for determining whether small molecule profiles are from the same individual, comprising:
- 20 obtaining one or more samples from an individual;  
determining the small molecule profiles of said samples;  
obtaining a tissue sample from an unknown source;  
determining the small molecule profile of the unknown source; and  
comparing the small molecule profiles, thus determining whether the
- 25 small molecule profiles are from the same individual.
55. A pharmaceutical composition comprising a small molecule identified by the method of claim 1.